

STP - Structure Search  
11/3/05

10/526,158

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ANSWER 1 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:74124 CAPLUS

DOCUMENT NUMBER: 142:156211

TITLE: Method for the preparation of highly pure 1-androstene derivatives with an oxidizing agent while maintaining pH control

INVENTOR(S): Moon, Young Ho; Kim, Dong Jun; Park, Chul-Hyun; Lee, Kyung Ik; Lee, Jae Cheol; Lee, Gwan Sun; Chang, Young-Kil

PATENT ASSIGNEE(S): Hanmi Pharm. Co., Ltd., S. Korea

SOURCE: PCT Int. Appl., 20 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005007670	A1	20050127	WO 2004-KR1786	20040719
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.:

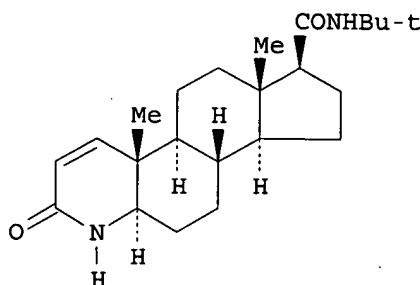
KR 2003-49529

A 20030719

OTHER SOURCE(S):

CASREACT 142:156211

GI



I

AB A method for preparing a 1-androstene derivative, I, which comprises reacting a 2-iodo-androstane derivative with an oxidizing agent while maintaining the pH of the reaction mixture at a specific range gives the 1-androstene derivative with high purity and yield.

IT 140700-61-4P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(method for the preparation of highly pure 1-androstene derivs. by treating a 2-iodo-androstane derivative with an oxidizing agent while maintaining the pH)

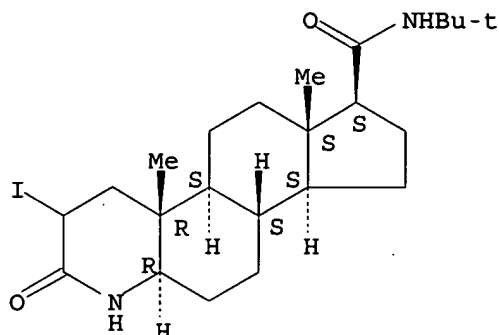
RN 140700-61-4 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-

10/526,158

dimethylethyl)hexadecahydro-3-iodo-4a,6a-dimethyl-2-oxo-,  
(4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 98319-26-7P 164656-23-9P

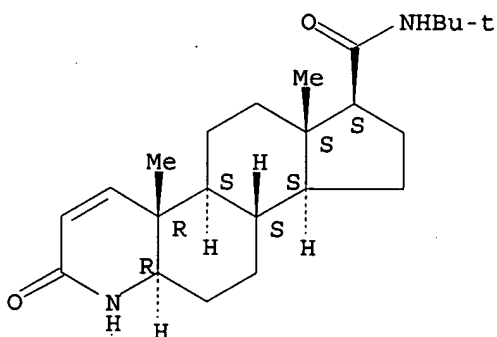
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP**  
(Preparation)

(method for the preparation of highly pure 1-androstene derivs. by treating  
a 2-iodo-androstane derivative with an oxidizing agent while maintaining  
the pH)

RN 98319-26-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-  
2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-,  
(4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

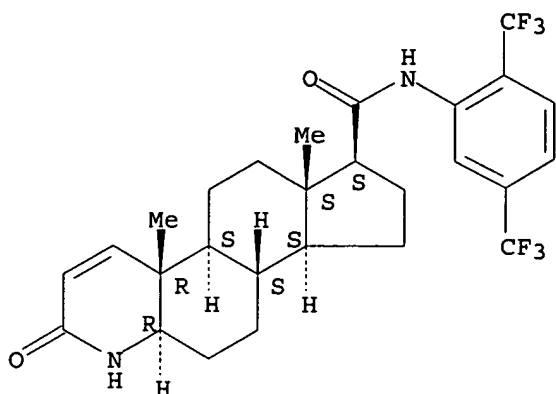
Absolute stereochemistry.



RN 164656-23-9 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-[2,5-  
bis(trifluoromethyl)phenyl]-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-  
tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI)  
(CA INDEX NAME)

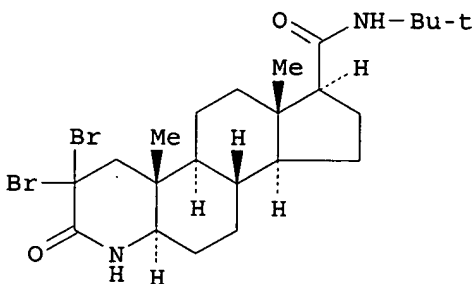
Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:399259 CAPLUS  
 DOCUMENT NUMBER: 140:375356  
 TITLE: Preparation of 2,2-dibromo-azasteroid and its use for introducing a 1,2-double bond into azasteroids  
 INVENTOR(S): Slemon, Clarke; Macel, Bob  
 PATENT ASSIGNEE(S): Torcan Chemical Ltd., Can.  
 SOURCE: Can. Pat. Appl., 32 pp.  
 CODEN: CPXXEB  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2271974	AA	20001114	CA 2000-2271974	19990514
PRIORITY APPLN. INFO.:			CA 2000-2271974	19990514
OTHER SOURCE(S):	CASREACT 140:375356; MARPAT 140:375356			



I

AB A process for introducing a 1,2-double bond into 17β-substituted-3-oxo-4-azasteroids includes the preparation of novel 2,2-dibromo-4-azasteroids by a three step process comprising oxalylation, reaction with excess bromine, and removal of the oxalyl group. This process is preferably carried out at temps. at or above -20°C and results in a high yield of the 2,2-dibromo-4-azasteroid. Thus, dibromodihydrofinasteride I was prepared from dihydrofinasteride. The 2,2-dibromo-4-azasteroid can be converted to the corresponding 17β-substituted-4-aza-5α-androst-

1-ene-3-one, finasteride, by at least two processes, one of which involves correcting the oxidation state at the 2-carbon and then introducing the 1,2-double bond, and the other of which involves introducing the unsatn. to produce a vinyl bromide followed by correcting the oxidation state of the 2-carbon. Preferably, the dibromo compound is reacted with thiophenol to produce a 2-phenylthio intermediate, followed by oxidation of the phenylthio group to a sulfoxide and 1,2-elimination of the sulfoxide group to create the 1,2- double bond.

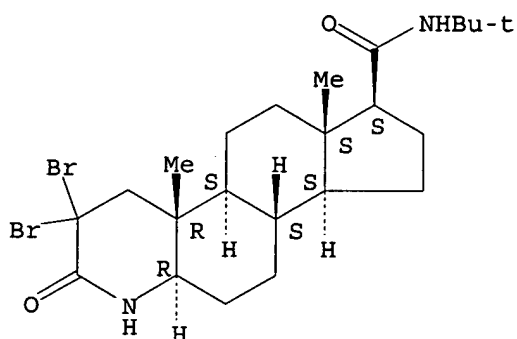
IT 684215-48-3P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of finasteride via dibromodihydrofinasteride)

RN 684215-48-3 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, 3,3-dibromo-N-(1,1-dimethylethyl)hexadecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



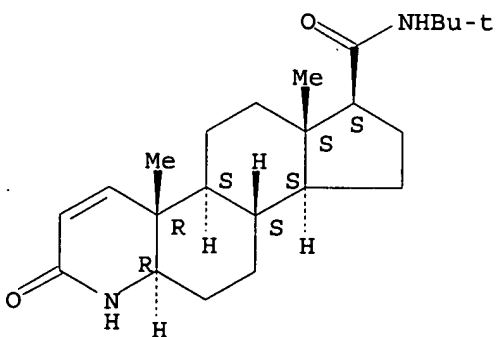
IT 98319-26-7P, Finasteride

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(preparation of finasteride via dibromodihydrofinasteride)

RN 98319-26-7 CAPLUS

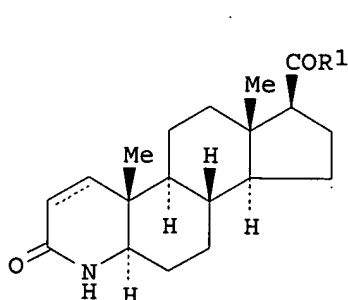
CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

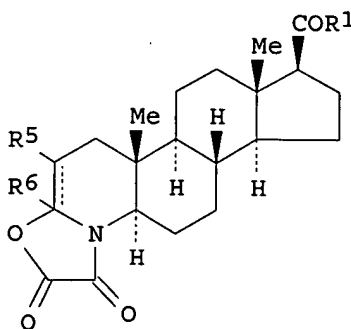


INVENTOR(S): oxo- $\Delta$ 1,2-4-azasteroids and intermediates thereof  
 Gorgojo Lobato, Jose Maria; Lorente Bonde-Larsen,  
 Antonio; Martin Juarez, Jorge  
 PATENT ASSIGNEE(S): Ragactives, S.L., Spain  
 SOURCE: PCT Int. Appl., 27 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Spanish  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003029267	A2	20030410	WO 2002-ES453	20020926
WO 2003029267	A3	20030619		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
ES 2185503	A1	20030416	ES 2001-2190	20010929
ES 2185503	B1	20040801		
CA 2461221	AA	20030410	CA 2002-2461221	20020926
EP 1437361	A2	20040714	EP 2002-779579	20020926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005504130	T2	20050210	JP 2003-532513	20020926
US 2004254209	A1	20041216	US 2004-810128	20040326
PRIORITY APPLN. INFO.:				
			ES 2001-2190	A 20010929
			WO 2002-ES453	W 20020926
OTHER SOURCE(S): CASREACT 138:287866; MARPAT 138:287866				
GI				



I



II

AB The present invention discloses a process for preparing 17 $\beta$ -substituted-3-oxo- $\Delta$ 1,2-4-azasteroids, such as I [R1 = alkyl, OR2; R2 = alkyl, NR3R4; R3, R4 = H, alkyl; dashed line = double bond], from 17 $\beta$ -substituted-3-oxo-4-azasteroids I [dashed line = single bond]. Thus, I [R1 = NHBu-t; dashed line = single bond] was reacted with oxalyl chloride to provide oxazolidinedione derivative II [R1 = NHBu-t; R5, R6 = H; dashed line = double bond], which upon reaction with 1,3-dibromo-5,5-dimethyl-hydantoin in presence of perchloric acid afford 2-bromo-3-hydroxyoxazolididione derivative II [R1 = NHBu-t; R5 = Br, R6 = OH;

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dashed line = single bond (III)]. III was reacted with potassium tert-butoxide in presence of anhydrous DMF to afford I [R1 = NHBu-t; dashed line = double bond]. Some prepared compds. are inhibitors of testosterone-5 $\alpha$ -reductase and can be used in the treatment of hyperandrogenic alterations.

IT 98319-26-7P, Finasteride 140852-02-4P

507221-54-7P

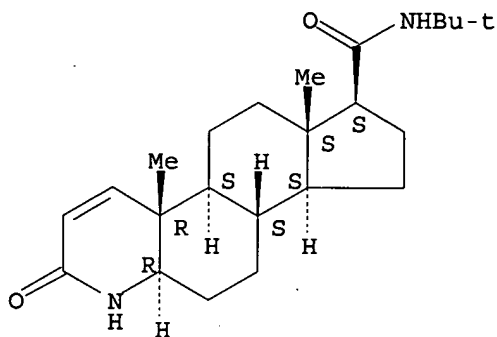
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 17 $\beta$ -substituted-3-oxo- $\Delta$ 1,2-4-azasteroids and intermediates thereof)

RN 98319-26-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

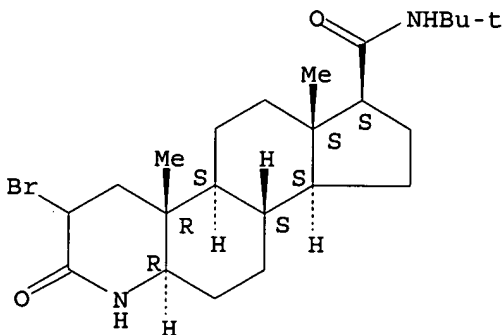
Absolute stereochemistry.



RN 140852-02-4 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, 3-bromo-N-(1,1-dimethylethyl)hexadecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

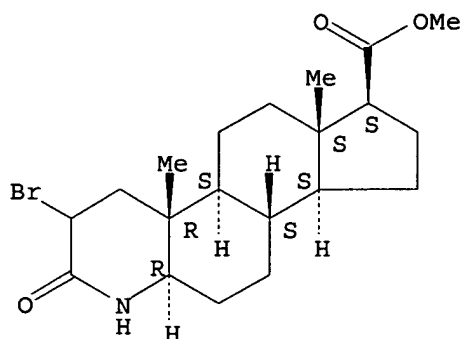
Absolute stereochemistry.



RN 507221-54-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxylic acid, 3-bromohexadecahydro-4a,6a-dimethyl-2-oxo-, methyl ester, (4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



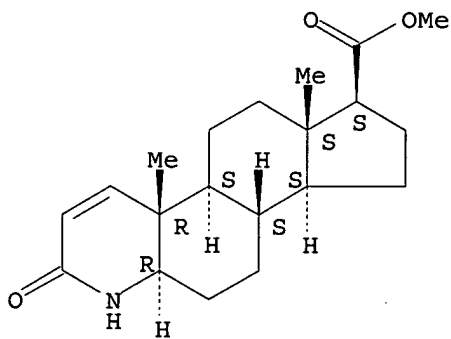
IT 103335-41-7P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP**  
(Preparation)(preparation of 17β-substituted-3-oxo-Δ1,2-4-azasteroids and  
intermediates thereof)

RN 103335-41-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxylic acid, 2,4a,4b,5,6,6a,7,8,9,9a,9b,10,  
11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, methyl ester,  
(4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:235962 CAPLUS

DOCUMENT NUMBER: 116:235962

TITLE: Process for iodinating or brominating the  
alpha-methylenic carbon of a secondary amideINVENTOR(S): King, Anthony On Ping; Abramson, Newton L.; Anderson,  
Kevin; Shuman, Richard F.; Karady, Sandor

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

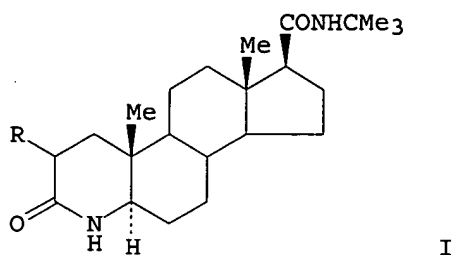
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 473225	A2	19920304	EP 1991-202133	19910821
EP 473225	A3	19931118		
EP 473225	B1	19970709		

R: CH, DE, FR, GB, IT, LI, NL

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US 5120847	A	19920609	US 1990-572920	19900827
CA 2049882	AA	19920228	CA 1991-2049882	19910826
CA 2049882	C	20020122		
JP 04261195	A2	19920917	JP 1991-215266	19910827
JP 06049674	B4	19940629		

PRIORITY APPLN. INFO.: US 1990-572920 A 19900827  
OTHER SOURCE(S): CASREACT 116:235962; MARPAT 116:235962  
GI



AB The  $\alpha$ -methylenic C of a secondary amide is halogenated by Br or iodine in the presence of a trialkylsilyl halide. Thus, androstane I (R = H) was treated with iodine in the presence of Me<sub>3</sub>SiCl and Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub> in PhMe to give I (R = iodo) quant. The latter compound was treated with KOtMe<sub>3</sub> in DMF to give 1-androstene.

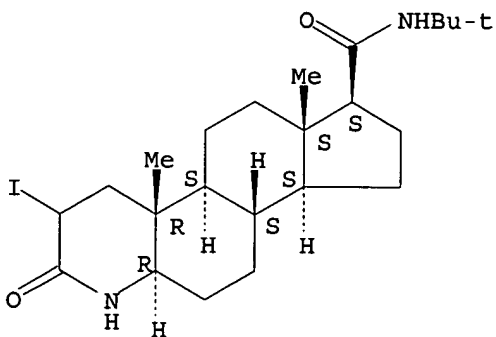
IT 140700-61-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and dehydroiodination of)

RN 140700-61-4 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)hexadecahydro-3-iodo-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 98319-26-7P

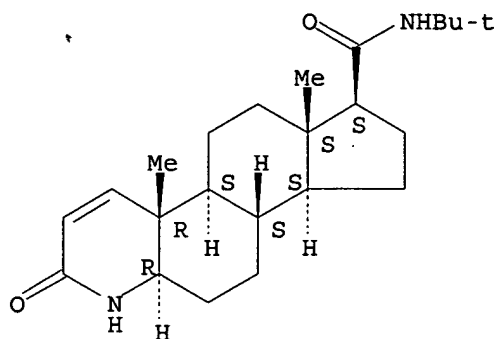
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 98319-26-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-, (4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:472017 CAPLUS

DOCUMENT NUMBER: 115:72017

TITLE: Method for introducing a 1,2 double bond into azasteroids

INVENTOR(S): King, Anthony O.; Weinstock, Leonard M.; Anderson, Kevin R.; Shuman, Richard F.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

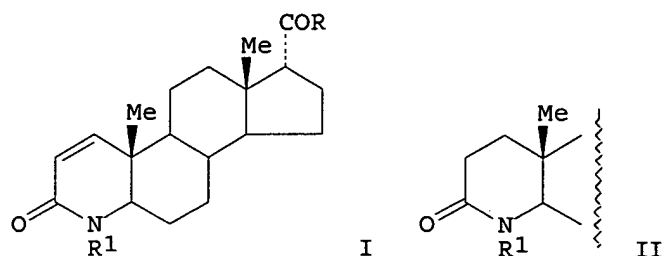
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 428366	A2	19910522	EP 1990-312341	19901113
EP 428366	A3	19920729		
EP 428366	B1	19950920		
R: CH, DE, FR, GB, IT, LI, NL				
US 5021575	A	19910604	US 1989-434663	19891113
CA 2029859	AA	19910514	CA 1990-2029859	19901113
CA 2029859	C	20020514		
JP 03206096	A2	19910909	JP 1990-304208	19901113
JP 06051718	B4	19940706		
EP 655459	A2	19950531	EP 1995-200326	19901113
EP 655459	A3	19960522		
EP 655459	B1	20000503		
R: CH, DE, FR, GB, IT, LI, NL				
LV 12572	B	20010420	LV 2000-117	20000907
PRIORITY APPLN. INFO.:			US 1989-434663	A 19891113
			EP 1990-312341	A3 19901113

OTHER SOURCE(S): CASREACT 115:72017; MARPAT 115:72017

GI



AB 1,2-Unsatd. azasteroids I [R = H, (un)substituted C1-12 alkyl, cycloalkyl, Ph, OH, alkoxy, OCH<sub>2</sub>Ph, amino; R<sub>1</sub> = H, Me, Et] were prepared from saturated derivs. II in a 3-step 1-pot reaction. Thus, II (R = CMe<sub>3</sub>, R<sub>1</sub> = H) was converted to oxazolidinedione derivs. with oxalyl chloride, brominated with Br, treated with MeNHCH<sub>2</sub>CH<sub>2</sub>OH to hydrolyze the oxazolidinedione, and dehydrobrominated with Me<sub>3</sub>COK. The overall yield of I (R = CMe<sub>3</sub>, R<sub>1</sub> = H) was 60.2%.

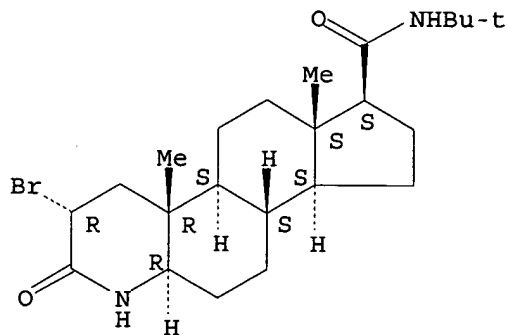
IT 135252-08-3P 135252-09-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and dehydrobromination of)

RN 135252-08-3 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, 3-bromo-N-(1,1-dimethylethyl)hexadecahydro-4a,6a-dimethyl-2-oxo-, (3R,4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

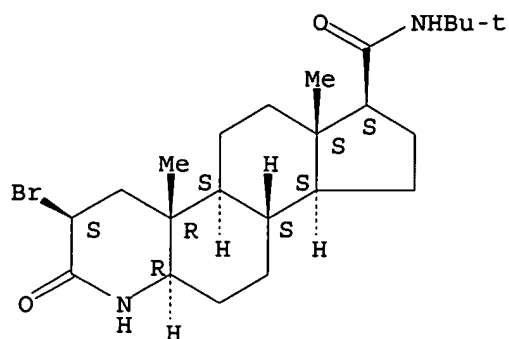


RN 135252-09-4 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, 3-bromo-N-(1,1-dimethylethyl)hexadecahydro-4a,6a-dimethyl-2-oxo-, (3S,4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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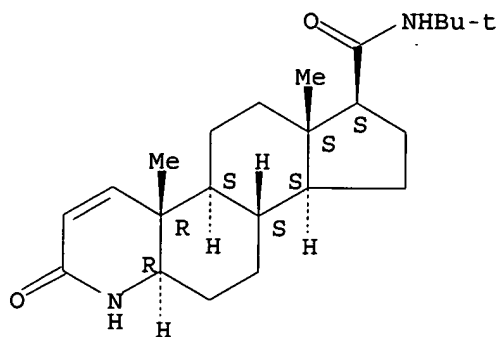
IT 98319-26-7P, MK906

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(preparation of, from 1,2-dihydro analog)

RN 98319-26-7 CAPLUS

CN 1H-Indeno[5,4-f]quinoline-7-carboxamide, N-(1,1-dimethylethyl)-  
2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-,  
(4aR,4bS,6aS,7S,9aS,9bS,11aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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(FILE 'HOME' ENTERED AT 09:38:58 ON 03 NOV 2005)

FILE 'REGISTRY' ENTERED AT 09:39:08 ON 03 NOV 2005

L1 STRUCTURE UPLOADED

L2 21 S L1

L3 336 S L1 FULL

L4 STRUCTURE UPLOADED

L5 1 S L4

L6 12 S L4 FULL

FILE 'CAPLUS' ENTERED AT 09:41:20 ON 03 NOV 2005

L7 117 S L3/PREP

L8 5 S L6/RCT

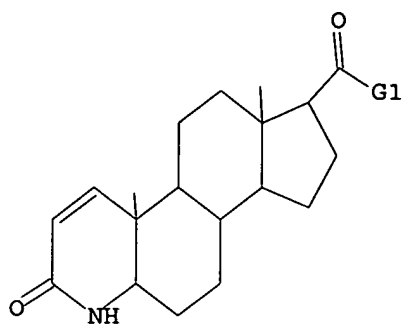
L9 5 S L7 AND L8

=> d l1

L1 HAS NO ANSWERS

L1 STR

10/526,158



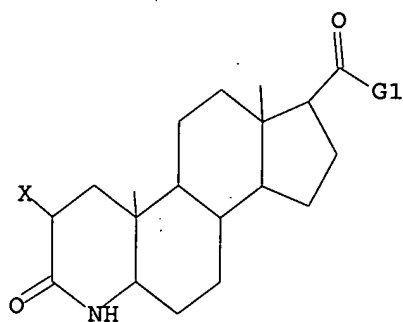
G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> d 14

L4 HAS NO ANSWERS

L4 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=>